

# Safety Data Sheet

# Benz[a]anthracene

Division of Safety  
National Institutes  
of Health



## WARNING!

THIS COMPOUND IS ABSORBED THROUGH THE SKIN AND RESPIRATORY AND INTESTINAL TRACTS. IT MAY IRRITATE TISSUES AND INDUCE SENSITIVITY. AVOID FORMATION AND BREATHING OF DUSTS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER. AVOID WASHING WITH SOLVENTS AND EXPOSURE TO UV LIGHT.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, INDUCE VOMITING. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF DUST. USE ORGANIC SOLVENT (NOT ALCOHOL) TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. CHECK FOR FLUORESCENCE OF RESIDUES WITH UV LIGHT. DISPOSE OF WASTE SOLUTIONS AND MATERIALS BY INCINERATION.

### A. Background

Benz[a]anthracene (BA) is not itself active as a carcinogen but is active with promoters such as phorbol esters. BA is a widespread environmental contaminant. It has no known commercial or industrial use and is employed solely in carcinogenesis research. It is destroyed through photooxidation in the atmosphere and is believed to be degraded slowly by bacteria in the soil.

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## B. Chemical and Physical Data

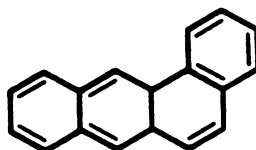
1. Chemical Abstract No.: 56-55-3

2. Synonyms:

BA	Benzo(a)phenanthrene	Tetraphene
1,2-Benzanthracene	2,3-Benzophenanthrene	Benzo(a)anthracene
Benzanthrene	2,3-Benzphenanthrene	Naphthanthracene

3. Molecular  
formula:  
 $C_{18}H_{12}$

structure:



weight:  
228.28

4. Density: No data.

5. Absorption spectroscopy: UV (Sadtler, 1961); UV and UV fluorescence (Schoental and Scott, 1949; Friedel and Orchin, 1951); IR (Sadtler, 1961; Fuson and Josien, 1956); MS (IARC, 1973); NMR (Bartle et al., 1969; Sadtler, 1961; Ozubko et al., 1974).

6. Vapor pressure:  $1.10 \times 10^{-7}$  mm Hg at 25°C (Radding et al., 1976). Sublimable.

7. Solubility: Soluble in most organic solvents; sparingly soluble in alcohol; solubility in water, 0.011 mg/liter.

8. Description, appearance: Colorless plates, yellow-green to violet fluorescence.

9. Boiling point: 400°C.

Melting point: 159-161°C.

10. Stability: Stable in dark at ambient temperature. Solutions undergo photooxidation in air and light.

11. Chemical reactivity: Not spontaneously reactive, but enters into numerous types of reactions with organic reagents.

12. Flash point: Does not apply.

13. Autoignition temperature: No data.

14. Flammable limits: Does not apply.

### Fire, Explosion, and Reactivity Hazard Data

1. BA does not require special fire-fighting procedures or equipment and does not present unusual fire and explosion hazards. Because of the electrostatic nature of dry BA, fire fighters should wear full-face masks.
2. BA is unstable in presence of light and is more unstable when UV radiation is present.
3. Incompatibilities: No data.
4. BA is not known to produce hazardous decomposition products.
5. BA is nonvolatile and does not require nonspark equipment. When handled in flammable solvents such as benzene, the precautions required for such solvents will apply. In powdered form BA is electrostatic, and when used in this form, it requires the use of antistatic devices.

### Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving BA.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by BA or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Wash surfaces with copious quantities of soap and water. Glassware should be rinsed (in a hood) with an organic solvent (not alcohol) followed by soap and water. Animal cages should be washed with soap and water.
3. Disposal: No waste streams containing BA shall be disposed of in sinks or general refuse. Surplus BA or chemical waste streams contaminated with BA shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (e.g., animal carcasses and bedding) containing BA shall be handled and packaged for incineration in accordance with the NIH

medical-pathological waste disposal system. Potentially infectious waste (e.g., tissue cultures) containing BA shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (e.g., absorbent bench top liners) minimally contaminated with BA shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (e.g., associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing BA shall be handled in accordance with the NIH radioactive waste disposal system.

4. Storage: Store solid BA and its solutions in dark-colored, tightly closed containers, preferably under refrigeration.

#### Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis (Jones and Freudenthal, 1978)

1. Sampling: Two methods are recommended: using an adsorption sampler in which cooled air is passed through Tenax and using high-volume filtration through fiberglass filter traps.
2. Separation and analysis: Several methods are available and offer various degrees of sensitivity. For separation, TLC, HPLC, and GC are useful. TLC is the least efficient of these three methods. HPLC and GC are highly efficient. The most useful and sensitive method for separation and analysis of BA is GC-MS. This method allows for accurate identification in the nanogram to picogram level; it is still desirable to confirm the identification by other analytical methods. UV spectroscopy is useful but is limited because of possible similarity in spectra with related compounds. Fluorescence spectroscopy gives both excitation and emission spectra, and its sensitivity level is in the nanogram range. It is more sensitive than UV by a factor of  $10^2$  or  $10^3$  or greater. Other methods are phosphorescence, NMR, and IR spectroscopy.

#### Biological Effects (Animal and Human)

1. Absorption: BA is readily absorbed through the skin and by intravenous and intraperitoneal injection, ingestion, and inhalation (IARC, 1973).
2. Distribution: No data available; however, by comparison with the chemically and physically similar benzo[a]pyrene, it may be assumed that orally or parenterally administered BA accumulates quickly in almost all tissues. Among major organs involved are liver, intestines, skin, respiratory system, kidney, spleen, and bladder.

3. Metabolism and excretion: BA is metabolized by liver microsomes and liver and lung homogenates, through the action of aryl hydrocarbon hydroxylase(s) (AHH), to a variety of epoxides, diols, phenols, and quinones (Boyland and Sims, 1964). It is these oxidation products that are responsible for toxic and carcinogenic effects of BA. In analogy with benzo[a]pyrene, it is likely that diols are conjugated to glucuronides and epoxides to reduced glutathione, which would be excreted in the urine. No data substantiating this have been found for BA.
4. Toxic effects: There are no quantitative data on acute toxicity of BA; it is believed to be low in animals and man (Boyland et al., 1965; Heidelberger, 1975). It is perhaps significant that BA is only slightly toxic toward cultured hamster cells with low AHH activity but very toxic to cells with active AHH (Gelboin and Wiebel, 1971).
5. Carcinogenic effects: BA is weakly carcinogenic in experimental animals. Liver and lung carcinomas, and some stomach papillomas, have been noted in animals after repeated oral dosage with BA (IARC, 1973), and local tumors were produced by skin application to mice (Slaga et al., 1974) though not in rats and hamsters (IARC, 1973). In general, oxidation products of BA were more active in this respect than BA (Levin et al., 1978).
6. Mutagenic and teratogenic effects: BA is mutagenic to Drosophila, Salmonella mutants, and various rodent cells in vitro after metabolic activation. There are no data concerning its teratogenicity.

### Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. Skin should not be rinsed with organic solvents or scanned with UV light. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician.

### References

- Bartle, K.D., D.W. Jones, and R.S. Matthews. 1969. High field nuclear magnetic resonance of some carcinogenic polynuclear hydrocarbons. *Spectrochimica Acta* 25A:1603-1613.

- Boyland, E., and P. Sims. 1964. Metabolism of polycyclic compounds: The metabolism of benz[a]anthracene. *Biochem J* 91:493-506.
- Boyland, E., P. Sims, and C. Huggins. 1965. Induction of adrenal damage and cancer with metabolites of 7,12-dimethylbenz[a]anthracene. *Nature* 207:816-817.
- Friedel, R.A., and M. Orchin. 1951. *Ultraviolet Spectra of Aromatic Compounds*. John Wiley and Sons, New York.
- Fuson, N., and M.L. Josien. 1956. Infrared spectra of polynuclear aromatic compounds. I. 1,2-Benzanthracene, the monomethyl-1,2-benzanthracenes and some dimethyl-1,2-benzanthracenes. *J Am Chem Soc* 78:3049-3060.
- Gelboin, H.U., and F.J. Wiebel. 1971. Mechanism of aryl hydrocarbon hydroxylase induction and its role in cytotoxicity and tumorigenicity. *Ann NY Acad Sci* 179:529-547.
- Heidelberger, C. 1975. Chemical carcinogenesis. *Annu Rev Biochem* 44:79-121.
- IARC, International Agency for Research on Cancer. 1973. *Mono-graph on the evaluation of carcinogenic risk of the chemical to man: Certain polycyclic aromatic hydrocarbons and heterocyclic compounds, Vol. 3*. World Health Organization, Geneva, Switzerland.
- Jones, P.W., and R.I. Freudenthal, eds. 1978. *Carcinogenesis, Vol. 3*. Raven Press, New York.
- Levin, W., D.R. Thakker, A.W. Wood, R.L. Chang, R.E. Lehr, D.M. Jerina, and A.H. Conney. 1978. Evidence that benzo[a]anthracene 3,4-diol-1,2-epoxide is an ultimate carcinogen on mouse skin. *Cancer Res* 38:1705-1710.
- Ozubko, R.S., G.W. Buchanan, and I.C. Smith. 1974. Carbon-13 nuclear magnetic resonance spectra of carcinogenic polynuclear hydrocarbons. I. 3-Methylcholanthrene and related benzanthracenes. *Can J Chem* 52:2493-2501.
- Radding, S., B.T. Mill, C.W. Gould, D.H. Liu, H.L. Johnson, D.C. Bomberger, and C.V. Fojo. 1976. *The Environmental Fate of Selected Polynuclear Aromatic Hydrocarbons*. Environmental Protection Agency (EPA), Washington, DC. 560/5-75-009.
- Sadtler Standard Spectra. 1961. Sadtler Research Laboratories, Inc., Philadelphia, PA.

al, R., and E.J. Scott. 1949. Fluorescence spectra  
of polycyclic aromatic hydrocarbons in solution. J Chem  
83-1696.

T.J., G.T. Bowden, J.D. Scribner, and R.K. Boutwell.  
Dose-response studies on the ability of 7,12-dimethylbenz[a]  
anthracene and benz[a]anthracene to initiate skin tumors.  
Cancer Res. 50: 1007-1010.